Getting Started in CASREACT®

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GETTING STARTED IN CASREACT

GENERAL INFORMATION

When you need reaction information, use CASREACT on STN®. This booklet gives you a brief overview of what is available in CASREACT for answering your reaction questions.

DATABASE CONTENT

CASREACT, the Chemical Abstracts Reaction Search Service, offers you easy access to current reaction information found in literature covering synthetic organic chemistry. The literature includes journals and patents from 1840 to the present. In late 2010, the database contained more than 1,231,900 records. In these records, you will find in-depth reaction and condition information on more than 22.7 million single- and multi-step reactions. New information is added to the database on a weekly basis.

LEARNING DATABASE

To assist new CASREACT searchers, the LCASREACT[SM] learning database contains a fixed number of documents with single- and multi-step reactions. All the search and display features found in CASREACT are available in LCASREACT, and there are no search or display fees in LCASREACT. Therefore, LCASREACT is a good place to practice reaction searching techniques and to familiarize yourself with display features.

SEARCH OPTIONS

CASREACT offers quick retrieval of answers to your reaction questions with a variety of search options. You can look for reaction information by using:

- Reaction participant structures
- CAS Registry Numbers®
- Functional groups
- Functional group class terms
- Special reaction terms such as yields
- Bibliographic terms
- Search results from other STN databases

Indexes, abstracts, and bibliographic information are also searchable and offer an easy way to refine your search results. For example, you can restrict the answers to work being done by a specific company or to papers published within the past year.

REACTION QUERIES

In CASREACT, you can specify many things about substances that participate in a reaction:

- Specify the role you want a substance to play in the reaction
- Mark reaction sites
- Indicate atom mapping through the reaction
- Require that a reaction include specific solvents and/or catalysts

STN INTERFACES

STN Express® and STN® on the Web[SM] make it easy to construct a reaction query made up of the structures for the reactants and/or products.

You can easily draw the reaction scheme with these tools just as you would sketch it in your notebook. Then, log on to STN and upload and search the reaction query. An example is provided later in the *Reaction Structure Searching* section.

LOOKING AT ANSWERS

CASREACT offers a variety of ways to look at the answers to your reaction questions. By default, you see a compact display of the first reaction that fits your search query in the most recent document retrieved, i.e., the first hit reaction. The structure diagrams of the reactants and products are shown with reagents, solvents, catalysts, and reaction conditions noted on the reaction arrow. The source and publication year are included in the display.

You can alternatively scan some of the answers to see if your search is on target. Scanning is free, and you can see the title of the paper and the compact display of the first hit reaction.

Complete records with all the bibliographic information, abstracts, indexing, and all the single-step reactions can also be displayed. You can view your answers online or have them delivered to you.

ADDITIONAL INFORMATION

In this booklet, we illustrate the various ways of answering your reaction information needs. More information is readily available by referring to:

- CASREACT Database Summary Sheet (www.cas.org)
- *CASREACT User Guide* (www.cas.org)
- *STN Express User Guide* (www.cas.org)
- STN on the Web Search Assistants (stnweb.cas.org)
- *Building and Searching Structures on STN* (available upon request from the CAS Customer Center)

In addition, extensive help messages are available while you are online:

- => HELP DIRECTORY in CASREACT for a list of help messages
- => HELP SFIELD to see the available search fields
- => HELP FORMAT to see the available display formats
- => HELP DFIELD to see the available display fields

STN HELP DESKS

- You can also get fast and friendly assistance from the experts at your STN Service Center's Help Desk. For contact information, visit: www.cas.org.

SEARCHING IN CASREACT

USING CAS REGISTRY NUMBERS

If you know the CAS Registry Numbers for reaction participants, it is very easy to retrieve reactions. Simply search the CAS Registry Number in the reaction role search fields. The available role search fields are:

- Reactant (/RCT)
- Product (/PRO)
- Reagent (/RGT)
- Reactant or Reagent (/RRT)
- Solvent (/SOL)
- Catalyst (/CAT)
- Nonproduct (/NPRO)
- Basic Index [all roles] (/BI or no qualification)

CAS REGISTRY NUMBER SEARCH OPTIONS

For a single reaction participant:

- Enter SEARCH (S) followed by the CAS Registry Number with /ROLE appended, e.g., => `S 50-00-0/RCT`.

For multiple reaction participants:

- Combine the /ROLE search terms with (L) proximity to search within the same single- or multi-step reaction, e.g., => `S 50-00-0/RCT (L) 110-88-3/PRO`.

Search Example

Find reactions that produce trioxane (110-88-3) from formaldehyde (50-00-0).

```
=> FIL CASREACT

=> S 50-00-0/RCT (L) 110-88-3/PRO
         19630 50-00-0/RCT
            33 110-88-3/PRO
L1          33 50-00-0/RCT (L) 110-88-3/PRO
```

After retrieving answers to your search, you can verify whether they meet your expectations at no charge by using D SCAN.

```
=> D SCAN

L1   33 ANSWERS   CASREACT   COPYRIGHT 2010 ACS on STN

TI   preparation of trioxane via trimerization of formaldehyde
     in the presence of polyalkylene glycol
 RX(1) OF 3

              H2C══O     H2SO4, (HOCH2CH2)2O,
                         Water

 NOTE: reaction mixt. was evapd. for 20 h
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
```

Once you are satisfied that the results meet with your expectations, you may display more detail by using the default DISPLAY (D) command. Entering simply "D" at a command prompt (=>) shows you the first hit reaction from the most recent retrieved citation to enter the database. The default display format (FHIT CRD) shows the compressed form of the reaction with additional detail, including the source information.

```
=> D

L1   ANSWER 1 OF 33   CASREACT   COPYRIGHT 2010 ACS on STN


 RX(1) OF 1

              H2C══O    Carbon, C:12027-38-2

 REF:  Jingxi Shiyou Huagong, 24(4), 29-33;  2007
 NOTE: solid-supported catalyst
```

The REF field shows the source information. The NOTE field adds detail about the reaction.

REFINING YOUR ANSWER SET

If you wish to further qualify your answer set, simply use the L-number of the answer set with additional terms.

- Use the (L) operator to limit the search with a single reaction sequence.
- Use the term ANY/CAT to include or exclude catalyzed reactions.
- Use the (NOTL) operator to eliminate specific reaction participants.
- Use 1/NS to limit the search to single-step reactions.
- The /NS field is a numeric field that specifies the number or range of reaction steps desired in your answers.

Search Example

Sulfuric acid (7664-93-9) is a common catalyst used in the preparation of trioxane from formaldehyde. Find reactions that use other catalysts.
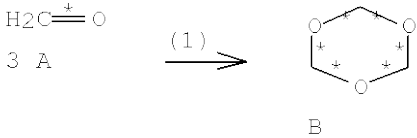
```
=> S L1 (L) ANY/CAT (NOTL) 7664-93-9/CAT
       306229 ANY/CAT
         6172 7664-93-9/CAT
L2         13 L1 (L) ANY/CAT (NOTL) 7664-93-9/CAT
```

To see the first hit reaction in the most recent retrieved citation with highlighted search terms, use the FHIT format. In this display, bonds that are partially or completely broken or formed in the reaction are indicated by an asterisk (*). Letters are used to indicate reactants, reagents, and products.

```
=> D FHIT

L2   ANSWER 1 OF 13  CASREACT   COPYRIGHT 2010 ACS on STN


RX(1) OF 1     3 A  ===>   B




  H2C===O
                  (1)
  3 A            ------>


                      B


RX(1)     RCT  A 50-00-0
          PRO  B 110-88-3
          CAT  7440-44-0 Carbon, 12027-38-2 Tungstate(4-),
               [µ12-[orthosilicato(4-)-
               κO:κO:κO:κO':κO':κO':κ
               O'':κO'':κO'':κO''':κO''':κO''']]t
               etracosa-µ-oxododecaoxododeca-, hydrogen (1:4)
          NTE  solid-supported catalyst
```

USING BIBLIOGRAPHIC SEARCH TERMS

The bibliographic, abstract, and indexing information (with the exception of the CAS Registry Numbers that are not part of indexed reactions) for a record is also searchable and may be combined with the reaction answer set. The Boolean operators AND, OR, and NOT may be used to combine these document record search terms with a reaction answer set.

Search Example

Did any of the trioxane synthetic papers come from Hoechst?

```
=> S L1 AND HOECHST/CS
          2346 HOECHST/CS
L3           3 L1 AND HOECHST/CS
```

Another option for viewing answers shows the bibliographic information in a compressed format along with the compressed display of the first hit reaction. This is the CBIB FCRD display format.

```
=> D CBIB FCRD

L3   ANSWER 1 OF 3  CASREACT  COPYRIGHT 2010 ACS on STN
121:83388  Process and catalyst for the gas-phase preparation of trioxane from
formaldehyde..  Emig, Gerhard; Krueger, Benno; Kern, Frank; Hoffmockel, Michael;
Mueck, Karl-Friedrich; Sextro, Guenter (Hoechst A.-G., Germany).  Eur. Pat. Appl.
EP 604884 A1 19940706, 9 pp.  DESIGNATED STATES:
R:  DE, ES, FR, GB, IT, NL.  (German).  CODEN: EPXXDW.
 APPLICATION: EP 1993-120599 19931221.  PRIORITY: DE 1992-4244582 19921231; DE
1993-4337706 19931105.


 RX(1) OF 1


                    H₂C══O     C:93280-40-1

 NOTE: steam-activated catalyst
```

SEARCHING WITH FUNCTIONAL GROUPS

CASREACT FUNCTIONAL GROUPS

Common reacting structural entities, called functional groups, may also be searched in CASREACT by using class or ring descriptions. The available search terms are derived from the structures of the reactants, reagents, and products.

To search using functional groups, enter the functional group term and its qualifying reaction role search field. The search fields allow you to specify not only that the structural feature is present in a reaction participant but also whether it is a reacting, forming, or nonreacting functional group. The available search fields are:

- Functional Group in Reactant (/FG.RCT)
- Functional Group in Product (/FG.PRO)
- Functional Group in Reagent (/FG.RGT)
- Reacting Functional Group (/FG.RXN)
- Forming Functional Group (/FG.FORM)
- Nonreacting Functional Group (/FG.NON)

The first three fields simply indicate that the functional group be present in the specified reaction participant. Use the last three fields to specify that a participant is reacting or forming or present, but not participating in the reaction.

FUNCTIONAL GROUP LIST

The list of valid search fields is available in the structure drawing window of STN Express or STN on the Web. The list may also be displayed online by entering HELP FGA (or HELP FGC for functional group classes) at a command prompt in CASREACT.

FUNCTIONAL GROUP SEARCH

To perform a functional group search, enter the SEARCH command followed by the functional group qualified with the appropriate role, e.g., => `S AMIDE/FG.RXN`.

To use more than a single reaction participant, combine the terms with (S) proximity to map the reacting atoms to the formed atoms.

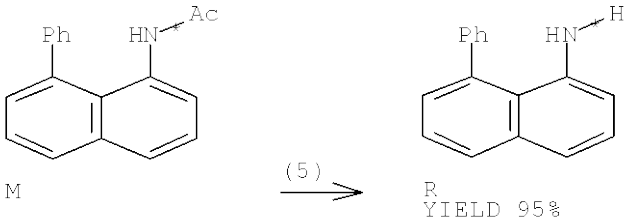---

Search Example

Find reactions that convert an amide to a primary amine.

```
=> S AMIDE/FG.RXN (S) PRIMARY AMINE/FG.FORM
        68601 AMIDE/FG.RXN
        71093 PRIMARY AMINE/FG.FORM
L1       7959 AMIDE/FG.RXN (S) PRIMARY AMINE/FG.FORM
```

The functional group terms are not displayable, but if you use a hit display format, the hit designations are highlighted. Examine the structure diagrams of the hit reaction participants for the functional groups that match the search question.

```
=> D FHIT
L1   ANSWER 1 OF 7959  CASREACT  COPYRIGHT 2010 ACS on STN


RX(5) OF 192      ...M  ===>  R...
```



```
RX(5)     RCT  M 25624-52-6

          STAGE(1)
             RGT  S 7647-01-0 HCl
             SOL  7732-18-5 Water, 64-17-5 EtOH
             CON  10 hours, reflux

          STAGE(2)
             RGT  T 1310-73-2 NaOH
             SOL  7732-18-5 Water, 60-29-7 Et2O
             CON  room temperature

          PRO  R 1254293-67-8
```

This answer is a two-stage reaction. The reaction map (M → R) and the reaction diagram (structures) show the initial reactant and the final product. The reaction summary (detail at the end of the display) shows all of the detail for both reaction stages.

NONREACTING FUNCTIONAL GROUPS

Use (L) proximity to link a nonreacting functional group into the reaction search. The (L) proximity keeps the additional terms within the same reaction sequence.

Search Example

Find reactions that convert amides to primary amines in the presence of a nonreacting carboxylate.

```
=> S AMIDE/FG.RXN (S) PRIMARY AMINE/FG.FORM (L)
     CARBOXYLATE/FG.NON
         68601 AMIDE/FG.RXN
         71093 PRIMARY AMINE/FG.FORM
        220654 CARBOXYLATE/FG.NON
L2         803 AMIDE/FG.RXN (S) PRIMARY AMINE/FG.FORM (L) CARBOXYLATE/FG.NON

=> D

L2   ANSWER 1 OF 803  CASREACT  COPYRIGHT 2010 ACS on STN

 RX(19) OF 850
```
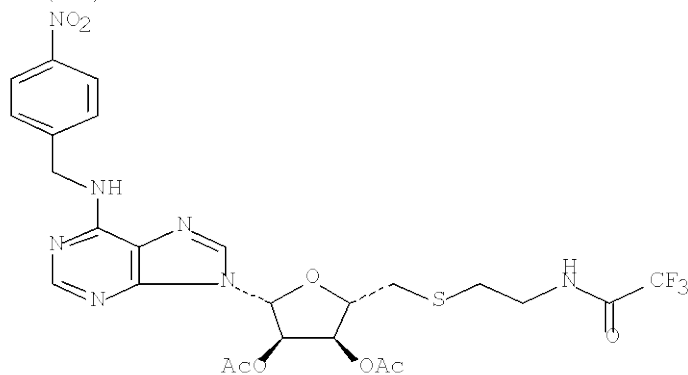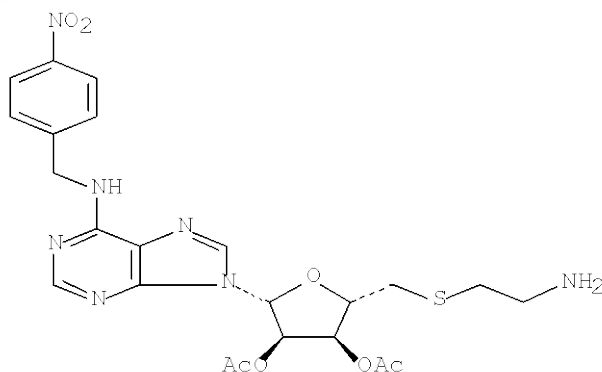
```
RX(19) OF 850
```



```
REF:   Journal of Medicinal Chemistry, 53(16), 6040-6053;  2010
NOTE:  sealed tube used
CON:   6 hours, 60 deg C
```

COST-EFFECTIVE SEARCHING

With functional group searching, plan your strategy so all of the functional group terms are included in a single search. You can add functional group search terms to an answer set, but that is billed as an additional functional group search.

REFINING YOUR ANSWER SET

You may use a functional group answer set L-number as a search term in further searching. The following illustrates the use of CAS Registry Number and bibliographic terms in combination with a functional group search.

USING FUNCTIONAL GROUPS AND CAS REGISTRY NUMBER

Functional groups can be combined with CAS Registry Number search terms either in the initial search or in a subsequent refinement step. Use the (L) operator to combine search terms.
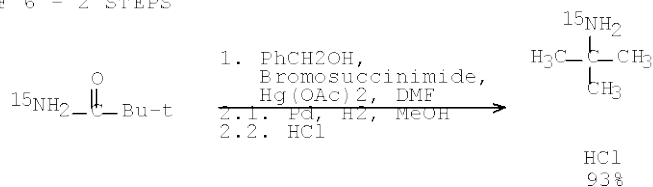
Search Example

Was palladium (7440-05-3) used as a catalyst in any of the reactions found in the amide-primary amine functional group search?

```
=> S L1 (L) 7440-05-3/CAT
        53686 7440-05-3/CAT
L3        806 L1 (L) 7440-05-3/CAT
=> D 1

L3   ANSWER 1 OF 806  CASREACT  COPYRIGHT 2010 ACS on STN
```

```
RX(5) OF 6 - 2 STEPS
                                                                  15NH2
                                                                   |
                                 1. PhCH2OH,                H3C___C___CH3
                                    Bromosuccinimide,              |
              O                     Hg(OAc)2, DMF                  CH3
     15NH2___C___Bu-t          2.1. Pd, H2, MeOH
                               2.2. HCl

                                                                  HCl
                                                                  93%
REF:   Journal of Labelled Compounds and Radiopharmaceuticals, 53(4),
       183-185;  2010
NOTE:  1) Hofmann rearrangement, in-situ generated catalyst (acetic
       acid), 2) overall yield 79% over 4 steps from pivaloyl chloride,
       HCl gas used in stage 2
CON:   STEP(1) 30 hours, room temperature
       STEP(2.1) 4 hours, room temperature; room temperature -> 0 deg C
       STEP(2.2) acidify
```

USING FUNCTIONAL GROUPS AND BIBLIOGRAPHIC TERMS

Functional group search terms or answer set L-numbers can be combined with bibliographic search terms or answer set L-numbers by using Boolean operators, AND, OR, or NOT.

Search Example

Are any of the reactions in L3 patents?
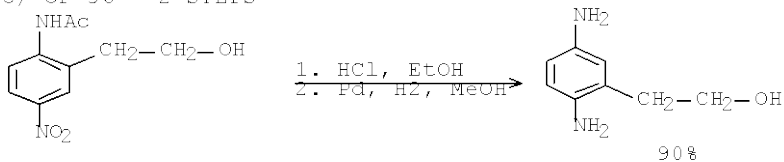
```
=> S L3 AND P/DT
        129421 P/DT
L4         244 L3 AND P/DT

=> D

L4   ANSWER 1 OF 244  CASREACT  COPYRIGHT 2010 ACS on STN

  RX(15) OF 36 - 2 STEPS
          NHAc
              CH2___CH2___OH                         NH2
                                   1. HCl, EtOH
                                   2. Pd, H2, MeOH        CH2___CH2___OH
          NO2                                        NH2
                                                        90%
  REF:   Faming Zhuanli Shenqing Gongkai Shuomingshu, 101698647, 28 Apr
         2010
  NOTE:  1) HCl gas used, 2) high pressure
  CON:   STEP(1.1) room temperature -> 75 deg C; 4 hours, 75 deg C
         STEP(2.1) room temperature -> 55 deg C, 1 MPa; 2 hours,
              50 - 55 deg C, 1 MPa
```

SEARCHING WITH FUNCTIONAL GROUP CLASS TERMS

CLASS TERMS

Broad classes of functional groups may also be used as search terms. When a class term is used in a search, STN automatically searches the specific functional groups included in the class term definition. For example, the class term KETONES automatically searches ACYCLIC KETONE, CYCLIC KETONE, O-QUINONE, and P-QUINONE.

CLASS TERM DEFINITION

The class term definitions may be found in the STN Express or STN on the Web structure drawing modules. You may also find it online by entering HELP FGC at a command prompt in CASREACT.

REACTION ROLES

Class terms may be searched in the same manner as functional group terms and in the same search fields. When combining more than one class term, use (S) proximity between terms to map the reacting group to the formed group. Use (L) proximity for nonreacting groups to keep all reaction participants within a single reaction sequence.
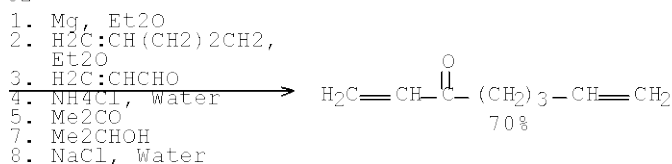

Search Example

Find studies that contain reactions that convert aldehydes to ketones.

```
=> S ALDEHYDE/FG.RXN (S) KETONES/FG.FORM
        140729 ALDEHYDE/FG.RXN
        115683 KETONES/FG.FORM
L1        9130 ALDEHYDE/FG.RXN (S) KETONES/FG.FORM

=> D
L1   ANSWER 1 OF 9130   CASREACT   COPYRIGHT 2010 ACS on STN
```

```
RX(1) OF 62
        1. Mg, Et2O
        2. H2C:CH(CH2)2CH2,
           Et2O                                    O
        3. H2C:CHCHO                               ||
        4. NH4Cl, Water   ────────>   H2C══CH─C─(CH2)3─CH══CH2
        5. Me2CO                                 70%
        7. Me2CHOH
        8. NaCl, Water
REF:  Advanced Synthesis & Catalysis, 352(11+12), 2057-2061;  2010
NOTE: fourth and sixth stages quenches; Jones oxidn. fifth stage
      stirred until a brownish-yellowish color remained, Grignard
      reaction, Jones reagent used
CON:  STAGE(1) room temperature
      STAGE(2) 1 hour, room temperature; room temperature -> -10 deg C
      STAGE(3) 30 minutes, -10 deg C; 30 minutes, -10 deg C
      STAGE(4) -10 deg C -> room temperature
      STAGE(5) room temperature -> 0 deg C
      STAGE(6) 0 deg C
      STAGE(7) 0 deg C -> room temperature
      STAGE(8) room temperature
```

REFINING YOUR ANSWER SET

These search results may also be refined with other types of CASREACT search terms.

Search Example

How many single-step catalyzed reactions were retrieved in L1?

```
=> S L1 (L) ANY/CAT (L) NS=1
      306229 ANY/CAT
      818690 NS=1
L2       1233 L1 (L) ANY/CAT (L) NS=1

=> D FHIT

L2   ANSWER 1 OF 1233  CASREACT  COPYRIGHT 2010 ACS on STN

RX(22) OF 22    AB  +  AN  ===>  AO
```
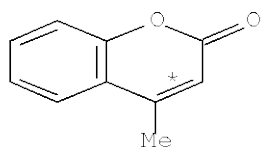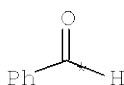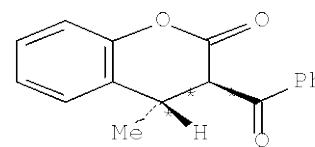


```
RX(22)
        STAGE(1)
          CAT  68986-76-5 Copper,
               (2-thiophenecarboxylato-κO2,κS1)-,
               866081-62-1 Quinoxaline,
               2,3-bis[(R)-(1,1-dimethylethyl)methylphosphino]-
          SOL  108-88-3 PhMe
          CON  10 minutes, room temperature
```

```
        STAGE(2)
           RGT  C 25015-63-8 1,3,2-Dioxaborolane, 4,4,5,5-tetramethyl-
           CON  10 minutes, room temperature

        STAGE(3)
           RCT  AB 607-71-6
           SOL  109-99-9 THF, 108-88-3 PhMe
           CON  SUBSTAGE(1) room temperature -> 40 deg C
                SUBSTAGE(2) 3 hours, 40 deg C
                SUBSTAGE(3) 40 deg C -> room temperature

        STAGE(4)
           RCT  AN 100-52-7
           CON  10 hours, room temperature

        STAGE(5)
           RGT  AP 26299-14-9 PCC
           SOL  75-09-2 CH2Cl2
           CON  room temperature

        STAGE(6)
           SOL  7732-18-5 Water
           CON  room temperature

      PRO  AO 1194476-52-2
      NTE  Schlenk tube; sixth stage quench, stereoselective
```

SEARCHING WITH SPECIAL REACTION TERMS

SPECIAL TERMS

There are several CASREACT reaction search fields that may be used for special searches or used to refine broad-based CAS Registry Number or structure searches in CASREACT.

- Number of Steps in a Reaction
- Yield Information
- Words in Reaction Notes

REACTION STEPS

You can specify a specific number of reaction steps or a range of reaction steps by using the Number of Steps (/NS) field. /NS is a numeric field and may be searched by using the spectrum of numeric operators. You can easily limit an answer set to single-step reactions by using NS=1 or 1/NS in your search logic. Use (L) proximity to combine the number of steps with other reaction search terms to restrict results to a single reaction sequence.

YIELD INFORMATION

Yield information may also be used as a search term. When the original document gives the yield for the product, it is included in the reaction information in the CASREACT record. The Yield (/YD) field is numeric and may be searched by using numeric operators. For further information, enter HELP YIELD at a command prompt in CASREACT.

Use (A) proximity to combine the yield information with a specific product, e.g.,
`=> S 138687-69-1/PRO (A) YD>=50.`

If you are searching with a functional group, enter the desired yield in the Functional Group Yield (/FG.YD) field. Use (A) proximity here as well,
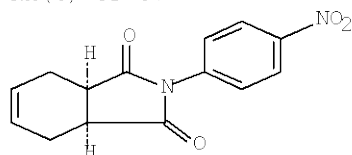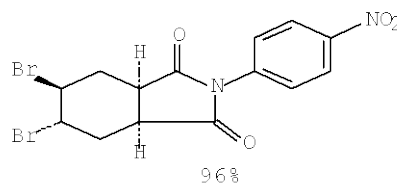e.g., `=> S NITRO/FG.FORM (A) 95-100/FG.YD.`

Search Example

Find high-yield (95-100%) preparations of products containing a nitro group.

```
=> S NITRO/FG.PRO (A) 95-100/FG.YD
         97979 NITRO/FG.PRO
        224276 95-100/FG.YD
L1       17350 NITRO/FG.PRO (A) 95-100/FG.YD

=> D
```

```
L1   ANSWER 1 OF 17350  CASREACT  COPYRIGHT 2010 ACS on STN

 RX(6) OF 57
```



```
 REF:   Azerbaidzhanskii Khimicheskii Zhurnal, (1), 43-52;  2010
 NOTE:  dropwise addition of aq. NaOCl, oxidative bromination with HBr/
        hydrogen peroxide in water or bromination with bromine in
        chloroform gave similar results, stereoselective
 CON:   STAGE(1) 1 hour, room temperature; 1 hour, room temperature
```

WORDS IN REACTION NOTES

The text displayed in the Reaction Notes (/NTE) field is searchable. You may even use left truncation and simultaneous left and right truncation on the search terms in the NTE field. Search terms in this field are combined with other reaction search terms by using (L) proximity to limit the results to a single reaction in the document record.

Search Example

Were any of the high-yield nitro preparations in L1 stereoselective?
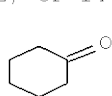
```
=> S L1 (L) ?STEREO?/NTE
       124636 ?STEREO?/NTE
L2       2631 L1 (L) ?STEREO?/NTE

=> D SCAN

L2   2631 ANSWERS   CASREACT  COPYRIGHT 2010 ACS on STN

TI   Enantioselective direct aldol reactions catalyzed by cinchonine-derived
prolinamides


 RX(12) OF 14
```
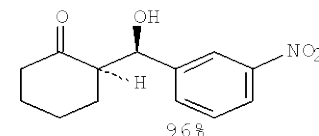


```
 NOTE: stereoselective, closed system used, aldol reaction, green
       chemistry - catalyst, no solvent, mechanism studied, R,2R:R,2S =
       1.4:1, 85% ee for R,2R isomer and 4% ee for R,2S isomer
```

SEARCHING WITH BIBLIOGRAPHIC SEARCH TERMS

DOCUMENT-BASED DATABASE

CASREACT also includes many types of bibliographic search terms for creating and refining reaction answer sets. If you do not qualify a search term, it is searched in the Basic Index, which contains single words from the title, abstract, supplementary terms, indexing terms, and reaction notes in the document record. The CAS Registry Numbers indexed for the document record are not searchable unless they are for an indexed reaction participant. Left truncation and simultaneous left and right truncation are available in the Basic Index.

BIBLIOGRAPHIC TERMS

The bibliographic terms offer a way to create an answer set that contains document information relevant to your reaction search.

Search Example

Find recent papers dealing with a Claisen rearrangement.

```
=> S CLAISEN REARRANG?
            5005 CLAISEN
               1 CLAISENS
            5005 CLAISEN
                    (CLAISEN OR CLAISENS)
           46287 REARRANG?
L1          3134 CLAISEN REARRANG?
                    (CLAISEN(W)REARRANG?)
```

Searches of this type can be used to create a small answer set to be combined with reaction search terms or to narrow the reaction search result. Use Boolean operators to combine bibliographic search results with reaction search results.
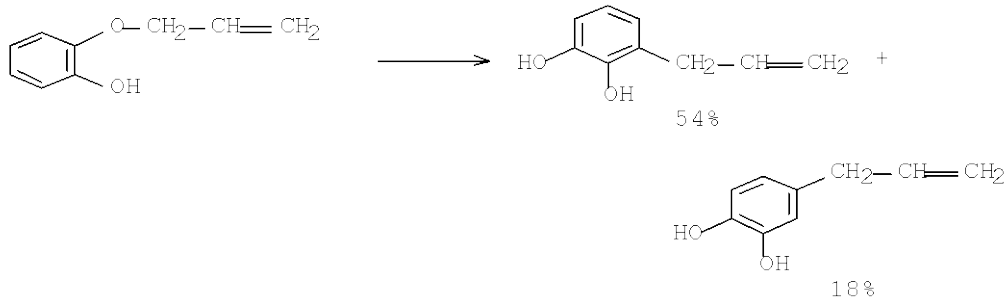
```
=> S L1 AND HETEROCYCLES/FG.RCT
                456355 HETEROCYCLES/FG.RCT
L2          1977 L1 AND HETEROCYCLES/FG.RCT

=> D SCAN

L2    1977 ANSWERS    CASREACT   COPYRIGHT 2010 ACS on STN

TI    Inhibitors of phosphatidylinositol-3-kinase (PI3) and inducers of nitric
oxide (NO)
```

```
RX(1) OF 132
```

NOTE: Claisen rearrangement

RCR RANGE SEARCHES

Reaction searches may be limited to the most recent two volumes of *Chemical Abstracts* by using the Recent Chemical Reactions (RCR) range setting.

```
=> S L2 RANGE=RCR
        22563 HETEROCYCLES/FG.RCT
L3         81 L1 AND HETEROCYCLES/FG.RCT

=> D 1 81 CBIB

L3   ANSWER 1 OF 81  CASREACT  COPYRIGHT 2010 ACS on STN
153:481291  Progress toward the Total Synthesis of (±)-Havellockate.
Beingessner, Rachel L.; Farand, Julie A.; Barriault, Louis (Department of
Chemistry, 10 Marie Curie, University of Ottawa, Ottawa, K1N 6N5, Can.). Journal
of Organic Chemistry, 75(19), 6337-6346 (English) 2010.  CODEN:
JOCEAH.  ISSN: 0022-3263.  Publisher: American Chemical Society.

L3   ANSWER 81 OF 81  CASREACT  COPYRIGHT 2010 ACS on STN
152:11983  Stereoselective synthesis of 11(E)-tetradecen-1-yl acetate-insect sex
pheromone of sod webworm (Loxostege sticticalis).  Shakhmaev, R. N.; Ishbaeva, A.
U.; Shayakhmetova, I. S. (Ufa State Oil Technical University,
Ufa, 450062, Russia).  Russian Journal of General Chemistry, 79(6), 1171-1174
(English) 2009.  CODEN: RJGCEK.  ISSN: 1070-3632.  Publisher: Pleiades
Publishing, Ltd..

=> D SCAN

L3   81 ANSWERS   CASREACT  COPYRIGHT 2010 ACS on STN

TI   Synthesis of 28-homobrassinosteroids modified in the 26-position
```
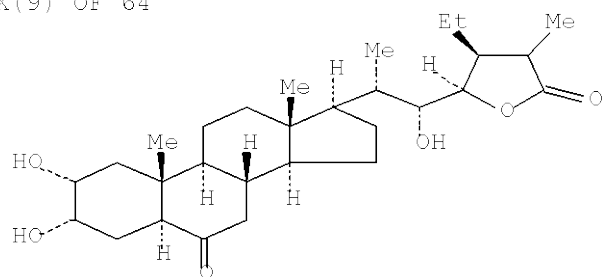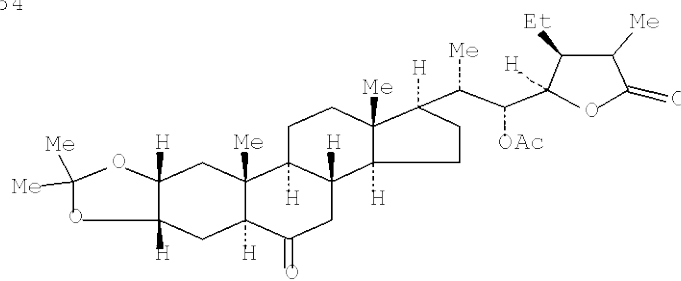
RX(9) OF 64

1. Me2CO, TsOH
2. Ac2O, Pyridine

(step 1)

RX(9) OF 64

57%

SEARCHING WITH ANSWER SETS FROM OTHER STN DATABASES

CROSSOVER SEARCHES

An answer set created in another STN database may be used as a search term in CASREACT. Simply create an answer set in an STN database, enter CASREACT, and search the answer set L-number from the initial search. The query from the initial search is automatically searched in CASREACT. For further information, enter HELP CROSSOVER at a command prompt.

COMBINE WITH REACTION SEARCH

A crossover answer set may be combined with a reaction search just like any other L-number. Did any of the reactions retrieved have pyridazines as reactants?

```
=> S L2 AND 1,2-C4N2/FG.RCT
          6445 1,2-C4N2/FG.RCT
L3           4 L2 AND 1,2-C4N2/FG.RCT

=> D TI FCRDREF

L3   ANSWER 1 OF 4  CASREACT  COPYRIGHT 2010 ACS on STN
TI   Preparation of aryltetrahydrobenzodiazepine derivatives and analogs as
norepinephrine, dopamine, and serotonin reuptake inhibitors
```



```
RX(1) OF 335
```
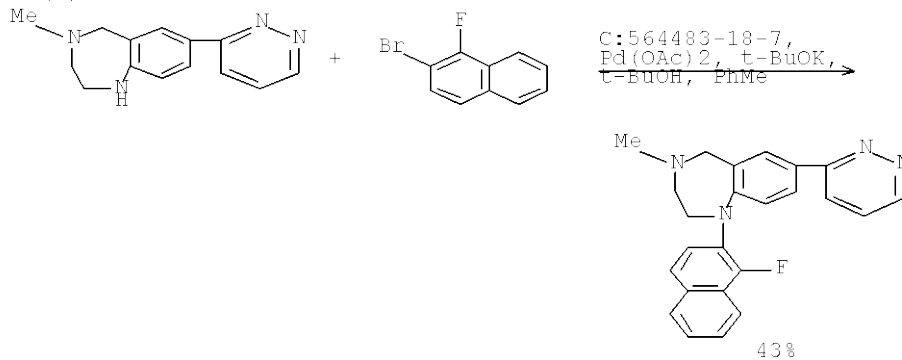
```
REF:  PCT Int. Appl., 2008141081, 20 Nov 2008
NOTE: microwave irradiation, chemoselective, Buchwald-Hartwig reaction,
      200 W used, sealed tube used
CON:  20 minutes, 120 deg C
```

SPECIAL TYPES OF CROSSOVER

There are two special types of crossover into CASREACT:

- Crossover from CA/CAplus (also HCA/HCAplus or ZCA/ZCAplus)
- Crossover from CAS REGISTRY

CA/CAplus Crossover

If you search an L-number from CA/CAplus in CASREACT, the Accession Numbers from the database are searched in CASREACT. For further details, enter HELP CACROSSOVER at a command prompt in CASREACT.

REGISTRY Crossover

If you search a REGISTRY L-number answer set in CASREACT, the CAS Registry Numbers contained in the answer set are searched. The L-number may be qualified with any of the reaction role search fields. This is a convenient way to search broad groups of compounds in the reaction search fields such as /CAT.

The term CASREACT appears in the Locator field (/LC) of every CASREACT substance found in REGISTRY. This term may be used to restrict the answer set to only those substances found in CASREACT prior to the actual crossover. Enter HELP RNCROSSOVER at a command prompt in CASREACT for further details.

Search Example

Find mercury-containing catalysts used in phenolic reactions.

```
=> FIL REGISTRY

=> S HG/ELS AND CASREACT/LC
          60197 HG/ELS
        7405727 CASREACT/LC
L1         7940 HG/ELS AND CASREACT/LC

=> FIL CASREACT

=> S L1/CAT (L) PHENOL/FG.RCT
           1129 L1/CAT
         112672 PHENOL/FG.RCT
L2           68 L1/CAT (L) PHENOL/FG.RCT

=> D SCAN

L2   68 ANSWERS   CASREACT   COPYRIGHT 2010 ACS on STN

TI   Reaction of 2,6-disubstituted phenols with vinyllead triacetates and alk-1-
ynyllead triacetates:  synthesis of 6-vinyl- and 6-alkynyl-cyclohexa-2,4-dienones
and crystal structure of 1,3,5,7-tetramethyl-3,5-bis(phenylethynyl)-
1,3,4,4a,5,8a-hexahydro-1,4-ethenonaphthalene-2,6-dione
```
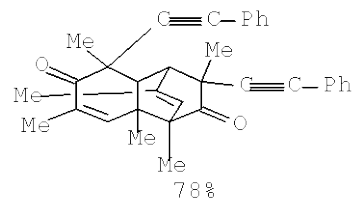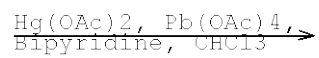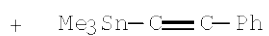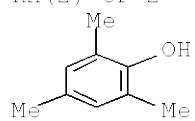
RX(2) OF 2

REACTION STRUCTURE SEARCHING

STRUCTURE QUERIES

All reactants, reagents, and products indexed in CASREACT are structure searchable. The structures may be drawn by using STN Express or the structure plug-in for STN on the Web. For complete details on drawing reaction participant structures, refer to:

- *STN Express User Guide* (www.cas.org)
- STN on the Web Search Assistants (stnweb.cas.org)

Structures may also be drawn by using the online STRUCTURE command. For details, refer to the *Building and Searching Structures in STN* manual, available from the CAS Customer Center: www.cas.org

For the following example, you need working knowledge of STN Express and its structure drawing module, as well as STN structure searching.

STEPS IN A REACTION STRUCTURE SEARCH

The example that follows uses STN Express. The reaction query may consist of up to four reaction participants.

This example looks for the reaction of a *p*-toluenesulfonyl chloride with a heterocyclic primary amine to form a sulfonamide.

| STEP	ACTION
1	Open STN Express and click **Prepare Query**.
2	Draw the reaction participants in the structure drawing window.
3	Add the reaction roles, reaction sites, and reaction map as desired.
4	Save the reaction query.
5	Enter CASREACT and upload the reaction query.
6	Run a SAMPLE search and examine the results.
7	Run a FULL search.
8	Refine your results.

Draw the Reaction Query

Open STN Express, and click the [Prepare Query] button. Draw all three reaction participants in the same window.
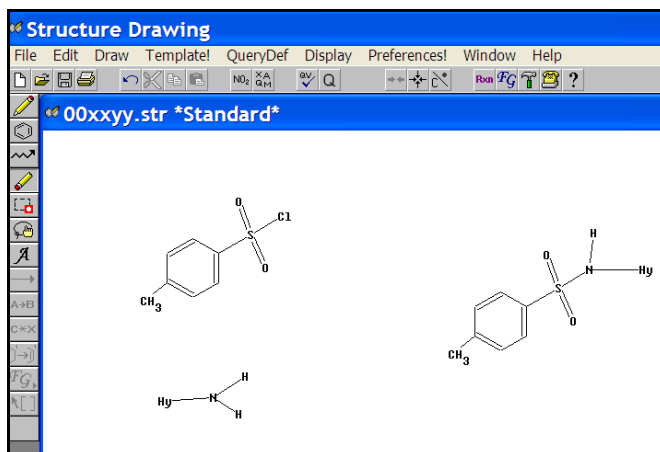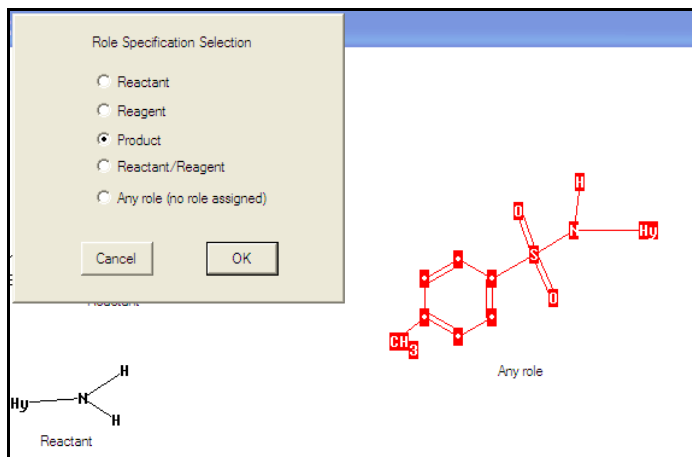

Add Reaction Roles

Click the [Rxn] button and assign reaction roles by clicking the **A→B** button and choosing the roles.
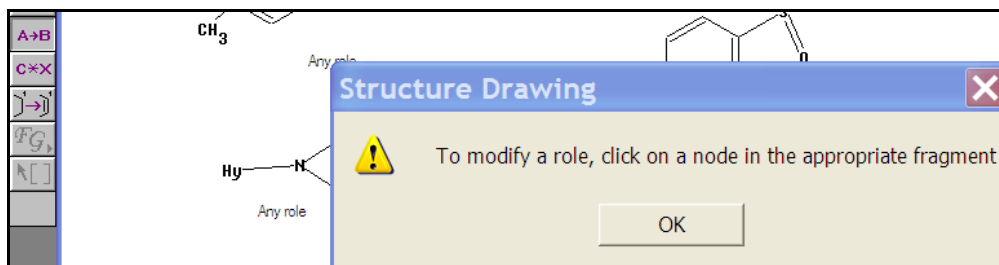
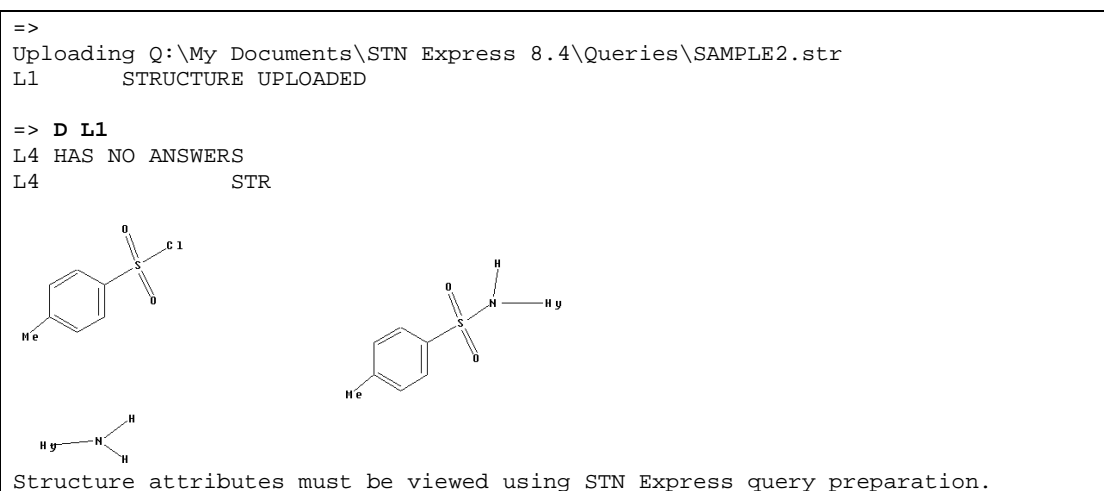Click on each participant and choose the appropriate reaction role.

Click **OK** after each selection. Save the reaction query.

Upload the Query

Enter CASREACT and upload the reaction query. You are prompted for the type of reaction database you are using. Take the default and click **OK**.

SAMPLE Search

Display the query to verify that it uploaded properly. Run a SAMPLE search.

```
=>
Uploading Q:\My Documents\STN Express 8.4\Queries\SAMPLE2.str
L1       STRUCTURE UPLOADED

=> D L1
L4 HAS NO ANSWERS
L4                 STR
```



```
Structure attributes must be viewed using STN Express query preparation.
```

```
=> S L1
SAMPLE SEARCH INITIATED 15:08:09
SCREENING COMPLETE -     8935 REACTIONS TO VERIFY FROM      314 DOCUMENTS


 56.0% DONE  5000 VERIFIED  42 HIT RXNS     8 DOCS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01


FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:    173046 TO    184354
PROJECTED ANSWERS:              94 TO        588


L2            8 SEA SSS SAM L1 (     42 REACTIONS)

The SAMPLE search (5% of total database) retrieved 8 document records with a
total of 42 hit reactions.  Use the no-fee D SCAN to examine answers.


=> D SCAN
L5    8 ANSWERS   CASREACT   COPYRIGHT 2010 ACS on STN

TI   Pyridazines. XXVII. Acylation reactions and procedures
     for regioselective alkylation of 5-amino-4-pyridazinyl
     aryl ketones
 RX(6) OF 46
```


FULL Search

Run the full reaction search and examine results.

```
=> S L1 FULL
FULL SEARCH INITIATED 15:08:57
SCREENING COMPLETE -   134937 REACTIONS TO VERIFY FROM     6038 DOCUMENTS

100.0% DONE  134937 VERIFIED  1296 HIT RXNS    368 DOCS
SEARCH TIME: 00.00.02

L3           368 SEA SSS FUL L1 (  1296 REACTIONS)

The full search found 368 documents with 1296 hit reactions.  Look at an answer
in the default display format.

=> D

L3   ANSWER 1 OF 368   CASREACT   COPYRIGHT 2010 ACS on STN
```
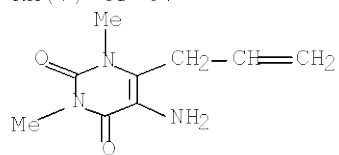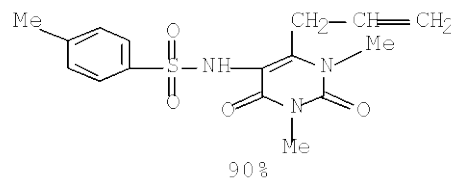
```
RX(7) OF 67

REF:   Synthesis, (8), 1315-1320;  2010
NOTE:  literature prepn.
CON:    - 2 hour, 80 deg C
```

Refining Results

Structure search results may be refined in the same way that other reaction searches are refined. Here we limit the answers to single-step reactions.

```
=> S L3 (L) NS=1
       818690 NS=1
L4        365 L3 (L) NS=1
```

Almost all of the retrieved answers contained a single-step hit reaction.

CONCLUSION

CASREACT offers you a wide variety of search methods that allow you to find the answers to your reaction questions by the means best suited to the question. Since CASREACT is a document-based database, you have access to bibliographic information as well as the synthesis information found in literature covering organic chemistry.

Once the answers have been obtained, you may view them by using any of the several available display formats that graphically display the reaction information, as well as the bibliographic, abstract, and indexing information.

CASREACT works very well in tandem with other STN databases, making your searches for reaction information efficient and cost effective.

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